Numerical Investigation of Waste-Heat Driven Adsorption Desalination Cycle

by

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Dissertation submitted in partial fulfillment of

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CERTIFICATION OF APPROVAL

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Approved by,

_____

(Dr Khairul Habib)

UNIVERSITI TEKNOLOGI PETRONAS

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May 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken by unspecified sources or persons.

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(Muhamad Fadzir Ab Razak)

ABSTRACT

Adsorption cycle is a practical and inexpensive method of desalinating the saline and brackish water to produce potable water for both industrial and residential applications. In recent years, many researcher has developed and experimented on the use of cost effective and environmental friendly adsorption cycle for desalination that require only low temperature waste heat to operate. Such waste heat is available in abundance from the exhaust of industrial processes, micro turbines of co-generation plants and renewable sources. Being waste heat driven, useful effects are generated by the adsorption desalination (AD) cycle with no additional burning of fuel and thus, mitigating the effects of global warming. Fundamental studies of adsorption, adsorption isotherm, kinetics and adsorbent used in the process of adsorption desalination were very importance to evaluate the cycle. With the implementation of adsorption-desorption phenomena, the cycle simultaneously produces high-grade potable water from a single heat input. In this proposal, it proposed the adsorption desalination (AD) system of two-bed operation mode that employs a low-temperature waste energy for numerically studies. The cycle will be calculated based on the utilization of waste heat sources in terms of mathematical modeling of a two-bed adsorption cycle based on adsorption isotherm, kinetics, mass and energy balances between the sorption elements, the evaporator and condenser. Then, the cycle will be monitored using key performance parameter namely (i) specific daily water production (SWDP), (ii) cycle time, and (iii) performance ratio (PR) for various heat sources temperature, mass flow rates, cycles times along with a fixed heat sink temperature. The numerical results of the adsorption cycle are validated using experimental data from the past researched.

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NOMENCLATURE

$\dot{m}$	Mass flow rate	ms^{-1}
c_p	Specific heat capacity	$J\ kg^{-1}\ K^{-1}$
D_{so}	A kinetic constant for the silica gel water system	$m^2\ s^{-1}$
E_a	Activation energy of surface diffusion	$Jmol^{-1}$
h	Enthalpy per unit mass	$J\ kg^{-1}\ K^{-1}$
h_{fg}	Latent heat	$kJ\ kg^{-1}$
K	The thermal conductivity	$W\ m^{-1}\ K^{-1}$
P	Pressure	Pa
PR	Performance ratio	
x	Fraction of refrigerant adsorbed by the adsorbent	$kg\ kg^{-1}$
Q	The total heat or energy W or J	
q*	The adsorbed quantity of adsorbate by the adsorbent under equilibrium conditions	$kg\ kg^{-1}$
ΔH_{st}	Isosteric heat of adsorption	$J\ kg^{-1}$
R	Universal gas constant	$J\ kg^{-1}\ K^{-1}$
R_p	Average radius of silica gel m	
SDWP	Specific daily water production	m^3/tonne-day
T	temperature	K
t	time / t/th-cycle	s
T_0	reference temperature	K
X	concentration of sea water	ppm

Subscripts

chilled	chilled water
cond	condenser
cw	cooling water
d	distillate
evap	evaporator
g	gas
hw	hot water
HX	heat exchanger
in	inlet
out	outlet
sg	silica gel

CHAPTER 1

INTRODUCTION

1.1 Background Study

1.1.1 Desalination and Adsorption desalination (AD)

Desalination refers to any of several processes that remove some amount of salt and other minerals from saline water. More generally, desalination may also refer to the removal of salts and minerals, as in soil desalination. Salt water is desalinated to produce fresh water suitable for human consumption or irrigation. One potential byproduct of desalination is salt. Desalination is used on many seagoing ships and submarines. Most of the modern interest in desalination is focused on developing cost-effective ways of providing fresh water for human use. Along with recycled wastewater, this is one of the few rainfall-independent water sources. Large-scale desalination typically uses large amounts of energy and specialized, expensive infrastructure, making it more expensive than fresh water from conventional sources, such as rivers or groundwater.

In Adsorption Desalination (AD), water is produced by the amalgamation of evaporation and condensation processes, which were triggered by adsorption and desorption of silica gel respectively. This water desalination technique is an innovative clean energy technology which can utilize waste heat/solar heat energy, saving huge amount of electric energy.

1.1.2 Problem Statement

The World Health Organization (WHO) reported that about 41% of the earth's population lives in "water-stressed" areas, and this water-deprived population is likely to climb to 3.5 billion in a decade or so. Thus, innovative and cost effective desalination technologies for producing fresh water are urgently needed. Most conventional and commercial-scale desalination plants have been built and operated and based on the evaporative and reverse osmosis methods. Such methods are energy

intensive, both electrically and thermally. Table 1.1 shows thermal and electric energy consumed for desalination processes [1].

Table 1.1: Thermal and Electric Energy Consumed for Conventional Desalination processes [1]

Method of Desalination	Thermal energy consumed kWh/m^3	Electric energy kWh/m^3 consumed	Primary fuel input kWh/m^3	Energy cost of water US$ per m^3
Multi-stage Flash	19.4	5.2	37.9	0.647
Multi-effect Distillation (MED)	16.4	3.8	30.5	0.52
Vapor Compression (VC)	_	11.1	29.2	0.497
Reverse Osmosis(RO) - single pass	_	8.2	21.5	0.366
Reverse Osmosis (RO) - double pass	_	9	23.7	0.403
Adsorption Desalination	Free	1.38	3.9	0.067

The total cost of water production in a desalination plant consists of more than the electricity consumption - electricity constitutes typically 25% of the overall cost whilst the other major costs include maintenance, membrane replacement, capital depreciation, etc.

In spite of the incremental improvements of the processes of desalination, which have contribute to the cost effectiveness and a sustainable production of fresh water, the conventional desalination plants are plagued by three major drawbacks [2] and they are (i) the high energy (primary or electricity) consumption of the plant, and the associated environmental emissions, (ii) erosion and blockage of materials of membranes and mass exchangers and (iii) high maintenance costs arising from salt deposition or fouling in the outer surfaces of heat exchangers as well as the corrosion of the tubes. Fouling and corrosion are known to escalate at high solution temperatures and the threshold for high salt deposition from the saline solution is known to occur when temperatures exceed 80 ^{0}C.

As compared with the commercial desalination methods, the adsorption technology has the unique advantages [3] such as (i) the utilization of the low-temperature waste heat, (ii) low corrosion and fouling rates on the tube materials due to the low temperature evaporation of saline water, (iii) and it has almost no major moving parts

which renders inherently low maintenance cost. In addition, the adsorption cycle offers two important benefits that are not available to the existing desalination technologies; namely, (i) a two-prong phenomenal barrier to any ‘‘bio-contamination’’ during the water generation process as compared with existing methods and (ii) the reduction in global warming due to the utilization of low-temperature waste heat which otherwise would have been purged to the atmosphere.

1.1.3 Objectives

The objectives of this project are of following:

- To conduct a numerical modeling and performance simulation of the waste heat driven AD cycle based on the literature.
- To evaluate the AD cycle performances and to optimize the operation of two bed configuration.

1.1.4 Scope of Study

- Adsorption desalination cycle using two or four-bed operation mode driven by waste heat.
- Energy balance of the evaporator, condenser and adsorber with respect to the heat sources temperature.
- Analyze the specific water production, cycle time, performance ratio (PR) for various heat sources temperature.

CHAPTER 2

LITERATURE REVIEW

2.1 Adsorption

Process that occur when a gas or liquid solute accumulates on the surface of a solid or a liquid (adsorbent), forming a molecular or atomic film (the adsorbate) was called adsorption. It is different from absorption, in which a substance diffuses into a liquid or solid to form a solution. The term sorption encompasses both processes, while desorption is the reverse process. Most natural physical, biological, and chemical systems are adsorption operative medium and is widely used in industrial applications such as activated charcoal, synthetic resins and water purification.

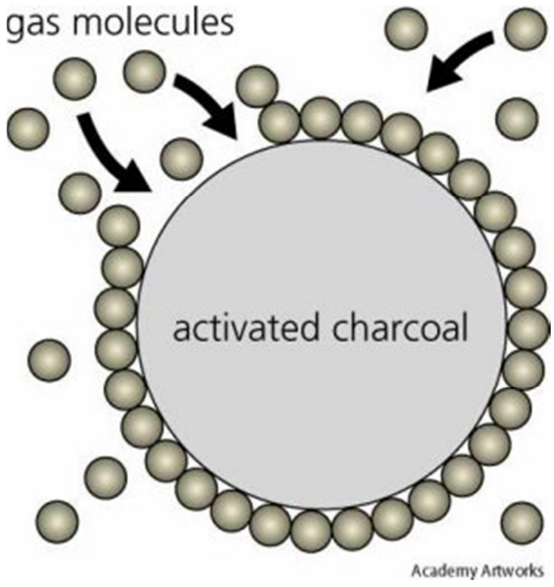


Figure 2.1 Adsorption on the surface of activated charcoal [4]

Similar to surface tension, adsorption is a consequence of surface energy. In a bulk material, all the bonding requirements (be they ionic, covalent or metallic) of the constituent atoms of the material are filled. But atoms on the (clean) surface experience a bond deficiency, because they are not wholly surrounded by other atoms. Thus it is energetically favourable for them to bond with whatever happens to

be available [5]. Depending upon the nature of forces existing between adsorbate molecules and adsorbent, the adsorption can be classified into two types [6]:

1. **Physical adsorption (physisorption):** Force of attraction existing between adsorbate and adsorbent are Vander Waal's forces. It is also known as Vander Waal's adsorption. In physical adsorption the force of attraction between the adsorbate and adsorbent are very weak, therefore this type of adsorption can be easily reversed by heating or by decreasing the pressure.

2. **Chemical adsorption (chemisorption):** Force of attraction existing between adsorbate and adsorbent are almost same strength as chemical bonds. It is also known as Langmuir adsorption. In chemisorption the force of attraction is very strong, therefore adsorption cannot be easily reversed. The extent of adsorption depends upon the following factors:

1. Nature of adsorbate and adsorbent.
2. The surface area of adsorbent.
3. Activation of adsorbent.
4. Experimental conditions. E.g., temperature, pressure, etc

2.2 Adsorption Isotherms

Adsorption isotherm known as a graph of adsorption processes. Basically, it shows graph between the amounts of adsorbate (x) adsorbed on the surface of adsorbent (m) and pressure at constant temperature. Different adsorption isotherms have been Freundlich, Langmuir and BET theory.

2.2.1 Basic Adsorption Isotherm

In the process of adsorption, adsorbate gets adsorbed on adsorbent [7].

$$\text{Adsorbate} + \text{Adsorbent} \underset{\text{desorption}}{\overset{\text{Adsorption}}{\rightleftharpoons}} \text{Adsorption}$$

$$A + B \rightleftharpoons AB$$

According to Le-Chatelier principle, the direction of equilibrium would shift in that direction where the stress can be relieved. In case of application of excess of pressure to the equilibrium system, the equilibrium will shift in the direction where the number of molecules decreases. Since number of molecules decreases in forward direction, with the increases in pressure, forward direction of equilibrium will be favored.

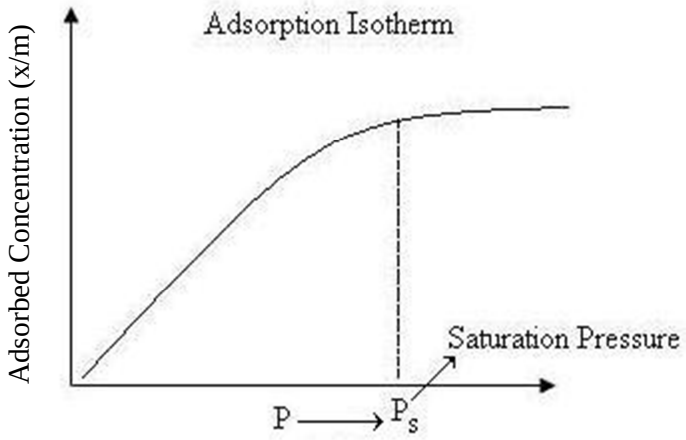


Figure 2.2: Basic Adsorption Isotherm

From the Figure 2.2, we can predict that after saturation pressure P_s, adsorption does not occur anymore. This can be explained by the fact that there are limited numbers of vacancies on the surface of the adsorbent. At high pressure a stage is reached when all the sites are occupied and further increase in pressure does not cause any difference in adsorption process. At high pressure, adsorption is independent of pressure.

2.2.2 Freundlich Adsorption Isotherm

In 1909, Freundlich gave an empirical expression representing the isothermal variation of adsorption of a quantity of gas adsorbed by unit mass of solid adsorbent with pressure. This equation is known as Freundlich Adsorption Isotherm or Freundlich Adsorption equation or simply Freundlich Isotherm. Though Freundlich Isotherm correctly established the relationship of adsorption with pressure at lower values, it failed to predict value of adsorption at higher pressure.

2.2.3 Langmuir Adsorption Isotherm

In 1916 Langmuir proposed another Adsorption Isotherm known as Langmuir Adsorption isotherm. This isotherm was based on different assumptions one of which is that dynamic equilibrium exists between adsorbed gaseous molecules and the free gaseous molecules.

Based on his theory, he derived Langmuir Equation which depicted a relationship between the number of active sites of the surface undergoing adsorption and pressure. The basic limitation of Langmuir adsorption equation is that it is valid at low pressure only.

2.2.4 BET adsorption Isotherm

BET Theory put forward by Brunauer, Emmett and Teller explained that multilayer formation is the true picture of physical Adsorption.

One of the basic assumptions of Langmuir Adsorption Isotherm was that adsorption is monolayer in nature. Langmuir adsorption equation is applicable under the conditions of low pressure. Under these conditions, gaseous molecules would possess high thermal energy and high escape velocity. As a result of this less number of gaseous molecules would be available near the surface of adsorbent.

Under the condition of high pressure and low temperature, thermal energy of gaseous molecules decreases and more and more gaseous molecules would be available per unit surface area. Due to this multilayer adsorption would occur. The multilayer formation was explained by BET Theory.

2.3 Adsorption Kinetics

The rate of adsorption of a molecule onto a surface can be expressed in the same manner as any kinetic process.

The rate of adsorption is governed by,

1. the rate of arrival of molecules at the surface
2. the proportion of incident molecules which undergo adsorption

We can express the rate of adsorption (per unit area of surface) as a product of the incident molecular flux and the sticking probability.The flux of incident molecules is given by the Hertz-Knudsen equation.

The sticking probability is clearly a property of the adsorbate / substrate system under consideration but must lie in the range $0 < S < 1$. It may depend upon various factors.

2.4 Adsorption Characteristics of Silica Gel–Water Pair

2.4.1 Physical Adsorption of Silica Gel

Silica gel is a partially dehydrated form of the polymeric colloidal silicic acid and its chemical composition is expressed as $SiO_2 \cdot nH_2O$. The adsorption/desorption equation for silica gel is given by

$$\mathbf{SiO_2 \cdot \mathit{n}H_2O\ (\mathit{s}) \leftrightarrows\ SiO_2\ (\mathit{n}\text{ -}1) \cdot H_2O\ (s) + H_2O\ (\mathit{g})} \qquad (2.1)$$

where *s* and *g* denote, respectively, solid phase and vapor phase. Commercially available silica gels are produced from silicate (20 wt% of SiO_2), the basic material in a sol–gel process that employs aluminum ions as a growth inhibitor for the primary silica gel. The production process of silica gel, as described by Ito et al [8], comprise the following:

(i) Reaction: Sodium silicate (SiO_2 – 20 wt%) + H_2SO_4, (ii) monomer, (iii) dimmer, (iv) particle, (v) silica solution (aqueous aluminum sulfate), (vi) three-dimensional gel network, (vii) pH_2 washing of aluminum sulfate, and (viii) drying.

Furthermore, silica gel can described as a dehydrated colloidal gel produced under controlled conditions from sulfuric acid and sodium silicate solution. Being chemically oxidized to silicon dioxide (SiO_2), it is made of an extremely hard and inert material which does not dust in service and it is quite inert when it comes into contact with most chemicals. The adsorptive action of silica gel for vapors is a physical effect and not a chemical reaction. The particles suffer no change in size or shape even when they are saturated with the adsorbate, and the particles appear

perfectly dry. The adsorptive property of the gel emanates from its high porosity, where the dimensions of the pores are sub-microscopic. The internal structure of silica gel has been proposed for the sorption behavior, that is, silica gel is described as a body with sub-microscopic pores piled together in a homogeneous mass. The pores are formed by the juxtaposition of silica particles with a distribution of sizes. Normal commercial silica gel will adsorb approximately 25–50% of its weight of adsorbate (water vapor) in a single component or mixture of saturated air. It has been estimated that 1 m^3 of adsorbent contains surface pores having a surface area of about $2.8x10^7$ m^2. This enormous internal surface and infinite number of small diameter capillaries attract vapors and hold them as "adsorbed phase" in the pores of capillaries. The weight of any compound adsorbed on silica gel depends on its partial pressure in the original gas mixture, the temperature of the silica gel and of the gas mixture, the compressibility and surface tension of the condensed liquid, its ability to wet the pore surface, and the volume and shape of the pores. Silica gel can adsorb vapor from a gas mixture until the pores of the gel are filled to a point where the internal vapor pressure of the adsorbed phase in the pores at a given temperature approaches as a limit the partial pressure of the vapor in the surroundings at the same temperature. The amount of an adsorbate that is adsorbed in silica gel at any gel temperature increases as the partial pressure of the vapor increases, and they would exist if the gas were "saturated" at the gel temperature. For example, silica gel at 28^0C in contact with air saturated at this temperature will adsorb an equilibrium uptake from 0.4 to 0.45 kg of water per kg of gel. As a result, increasing the temperature of the gel could result in a decrease in its adsorption capacity. Thus, it is clear that higher adsorption occurs with decreasing temperature. The maximum concentration of the vapor that is adsorbed occurs when the pores are saturated with vapor. In a reactivation process, silica gel would arrive at residual moisture content, and the useful concentration in the gel is the difference between the equilibrium concentration and the residual concentration under the conditions of use. Adsorption of an adsorbate liberates an equivalent amount of heat that is slightly greater than its latent heat of evaporation.

In order to regenerate silica gel, the amount of heat required varies with the design of the equipment, in addition to the supply of the heat necessary to release the adsorbed refrigerant from the gel, which is equivalent to the heat of adsorption. Heat must be

added for rising the temperature of the adsorbent bed and the adsorber, and to overcome heat leaks in the system. The action of silica gel is practically instantaneous under dynamic adsorption conditions, and the length of the adsorption period may be arbitrarily established [9].

The properties of silica gel are analysed using an AutoSorp-1 analyser. This instrument measures the amount of gas adsorbed or desorbed from a porous surface at a predetermined equilibrium (vapour) pressure by the static volumetric method with liquid Nitrogen at 77K as the filling fluid. The adsorption and desorption of N2 by different types of silica gels s observed that type RD-manufactured silica gel has the highest uptake. This type of adsorbent will be used in this investigation.

2.5 Desalination

Desalination has been a practical solution to the water shortage problems encountered in many countries of the world, in particular, in semi-arid regions as well as in countries with high population density. Over the decades, numerous commercial-scale desalination plants have been designed, built and operated [10], such as (i) the multi-stage flash (MSF) type, (ii) the multi-effect desalination type, (iii) the membrane-based reverse osmosis (RO) plants. More recent improvements include the hybrid plants, which combine the RO and MSF processes [11-16], could recover higher quality and yield of water with typical dissolved solids of less than 500 mg/l as required by the World Health Organization (WHO) standards. Ion exchange is another method whereby ions of dissolved inorganic salts are chemically replaced with the more desirable ions, and such a process has been used to minimize the fouling and carry-over to the water. Electro-dialysis (ED) or electro-dialysis reversal (EDR) [17] is deemed as one of the most promising techniques; however, the expected breakthrough has yet been realized. Recent development on adsorption desalination cycles is aimed to mitigate the short comings of the conventional desalination methods. The earliest patent related to adsorption-based desalination was reported by Broughton [18], using an ion-retarded resin for the vapor uptake, where a process with a thermally-driven two-bed configuration is simulated. Similar theoretical simulations of adsorption desalination plant were also proposed recently

by Zejli et al. [19] and Al-Kharabsheh and Goswami [20]. Solar heat source was studied as a heat source for the desalination plant, combined with an open-cycle adsorption heat pump using the Zeolite as the solid-vapor adsorbent. In another example, Richter [21] reported a similar solar-assisted desalination plant comprises an initial desorbed phase during the day and follows by an adsorption phase in the night hours. The long cycle time employed in the simulation yields a high coefficient of performance (COP) but being solar-driven, it is weather dependent. In this investigation, a unique two-bed adsorption desalination plant that employs a low-temperature waste energy was proposed and numerically studied. Figure 2.3 below shows the diagram of AD system in two-bed operation mode.

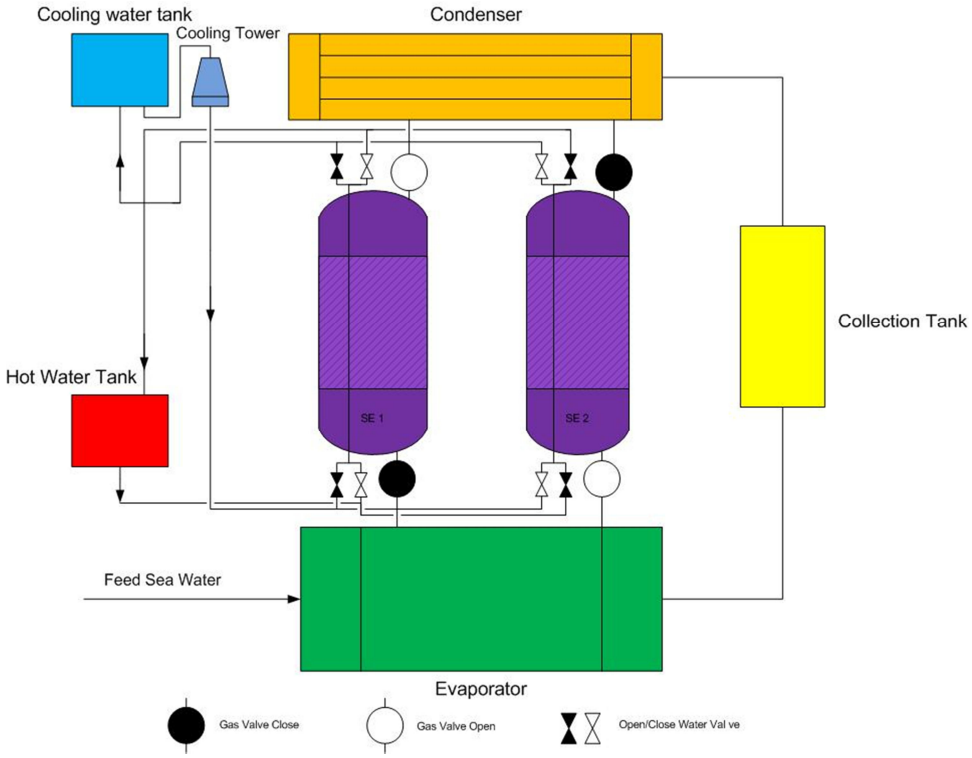


Figure 1.3: Skeletal diagram of AD system in 2-bed operation mode.

2.6 Adsorption desalination working principle

The cycle consists of three major components namely (a) the evaporator which is made of stainless steel or cupronickel to prevent corrosion, (b) the adsorber reactors where silica gel is packed around the heat exchanger tubes and (c) the condenser where the water vapor is condensed. The operation of the AD cycle can be described as follows:

(i) Sea or brackish water is pretreated using de-aeration method and is fed into the evaporator. The evaporator is the only unit which is made of anti-corrosive material such as cupronickel or stainless steel. A chilled water circuit is utilized to maintain the evaporation of the sea water. The outlet chilled water temperature ranges from 7 to 25^0C and it can be employed for cooling purposes. The spray water system is implemented to enhance the evaporation of feed water through flash evaporation. The sea or brackish water is sprayed at certain pressure into the evaporator whose pressure varies from 1.1 to 2.9 kPa depending on the chilled water supplied temperature.

(ii) The sea water level in the evaporator is regulated to maintain evaporation and control salt concentration. Concentrated brine from the evaporator is periodically purged for salt concentration control. In AD cycles, the evaporation occurs at low temperatures typically lower than 30^0C render.

(iii) The affinity for water vapor uptake by the unsaturated silica gel in the adsorber bed enhances the evaporation of the sea water. The water vapor from the evaporator is adsorbed on the surface of the silica gel inside the adsorber reactor. Cooling circuit is used to reject the heat of adsorption as well as maintain the adsorption process. The adsorption process continues until the preset cycle time is achieved.

(iv) The water vapor from the saturated silica gels (resulted from previous adsorption phase) is expelled from the adsorber using low temperature hot water.

(v) The desorbed vapors are condensed in the water-cooled condenser.

(vi) The condensate (fresh water) is collected in the collection tank which is either intermittently pumped out to the ambient or extracted via a 10 m high U-bend tube.

The numerical study was adapted from previous researched on a two and four-bed operation mode [22-24]. The specific water yield is measured numerically with respect to the key controlling parameters such as heat source temperatures, coolant temperatures, system switching and half-cycle operational time.

CHAPTER 3

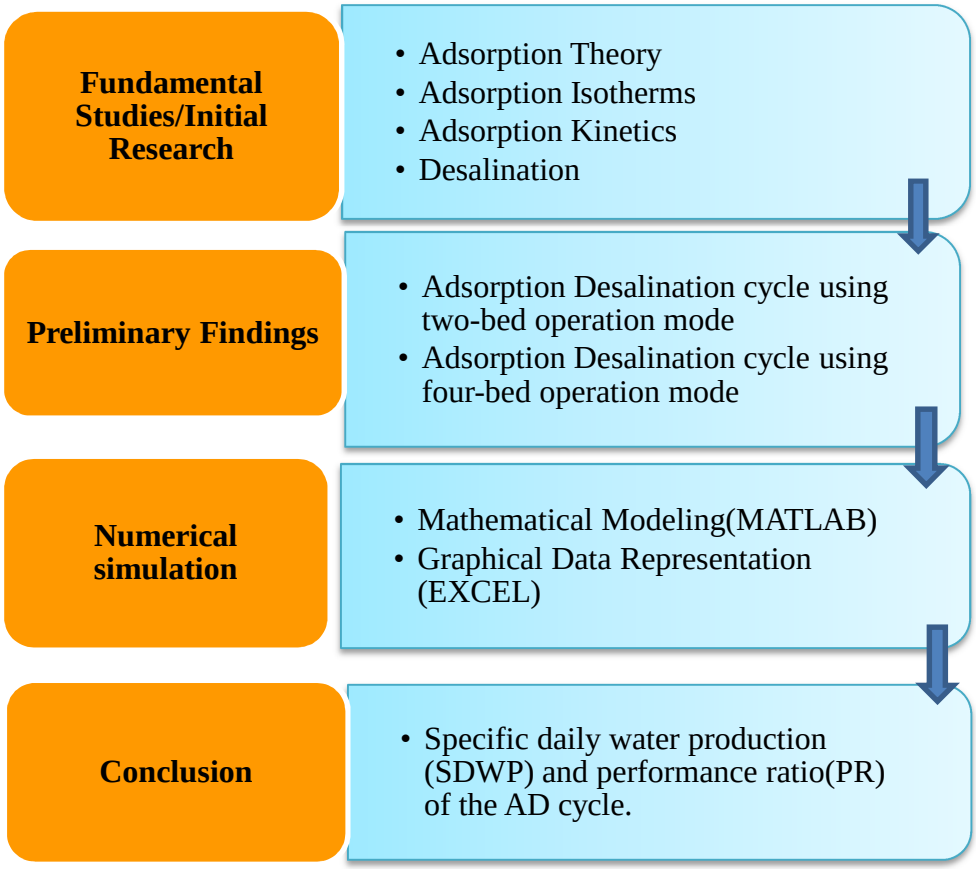
METHODOLOGY

This investigation is related with a cost-effective and environmentally friendly Adsorption (AD) cycle for desalination using waste heat. The adsorption cycle employs the adsorbate's affinity to an adsorbent, such as the silica gel and water pair, and operates in partial vacuum with no major moving parts.

The methodologies applied in this research include:

1) Fundamental studies on the adsorption and desorption characteristic of adsorbent-adsorbate pair.
2) Study on the advantages and disadvantages of Adsorption desalination process in producing potable water.
3) Performance analysis of the AD cycle using two-bed operational modes.
4) Mathematical modeling and graphical data representation.

3.1 Research Methodology Flow-Chart



3.2 Gantt Chart for FYP 2

No	Detail/Week	1	2	3	4	5	6	7	Semester Break	8	9	10	11	12	13	14	15	Remark
1	Project Work Continues																	Done
2	Submission of Progress Report																	Done
3	Project Work Continues																	Done
4	Pre-EDX																	Done
5	Submission of Draft Report																	Done
6	Submission of Dissertation (soft bound)																	
7	Submission of Technical Paper																	
8	Oral Presentation																	
9	Submission of Project Dissertation (Hard Bound)																	

CHAPTER 4

RESULT AND DISCUSSION

For developing equation in MATLAB, it is based on the adsorption isotherms, kinetics and energy balances between the sorption elements, the evaporator and the condenser and the type-RD silica gel is employed as the adsorbent. The parameters involve in this simulation was adapted from currently prototype facilities of Adsorption Desalination that located in National University of Singapore. All the properties of condenser, evaporator, adsorber and desorber were adapted in order to write the simulation program.

4.1 Mathematical Modeling

The following lumped parameter assumptions are made: (a) the temperature is uniform across the adsorbent (silica gel) layer; (b) the adsorption of the water vapor by the silica gel inside the adsorber bed is uniform; and (c) both the adsorbent (silica gel) and the adsorbate gas phases are in equilibrium condition in order to simplify the model.

The uptake of water vapor by the silica gel at temperature (T) and pressure (P) can be estimated using Freundlich Equation and adapted experimental data [26].

$$q^* = A(T_s) \times [P_s(T_w)/P_s(T_s)]^{B(T_s)} \quad (4.1)$$

where $P_s(T_w)$ and $Ps(T_s)$ are the saturation vapor pressure at temperatures *Tw* (water vapor) and *Ts* (silica gel) . The numerical values of *A*0 ~ *A*3 and *B*0 ~ *B*3 are determined by the least-square fit of experimental data and presented in the Appendix B.3.

The transient uptake of water vapor at specific temperature, pressure and adsorbate i.e., the kinetic of adsorption or desorption, is calculated by the linear driving force [27, 28] and this is given by,

$$\frac{\mathrm{d(t)}}{\mathrm{dt}} = K(q^* - x(t)) \tag{4.2}$$

where K is the mass-transfer coefficient. For a small range pressure regime (2 to 10 kPa), K is expressed in terms of key parameters R_p and D_{so} as [29].

$$K = \frac{15 D_{so}\, e^{-\frac{E_a}{RT}}}{R_p^2} \tag{4.3}$$

Where E_a is the activation energy of surface diffusion, R_p denotes the average radius of a silica gel particle, and D_{so} is the kinetic constant for the silica gel water system.

The inventory of the amount of sea water is fed into the evaporator and potable water is extracted from the condenser of the AD cycle and the mass balance of the cycle is thus given by

$$\frac{dM_{s,evap}}{dt} = \dot{m}_{s,in} - \dot{m}_{d,cond} - \dot{m}_b \tag{4.4}$$

Here, $M_{s,evaps}$ is the amount of sea water in the evaporator, $\dot{m}_{s,in}$ is the rate of feed sea water, $\dot{m}_{d,cond}$ is the mass of potable water extracted from the condenser and $\dot{m}_b$ is the mass of concentrated brine rejected from the evaporator. The feed sea water is intermittently pumped into the evaporator depending on the amount and level of sea water whilst brine is discharged once the concentration reaches to the predetermined limit.

The mass and salt balance for the evaporator of the AD cycle is given as

$$\frac{dM_{s,evap}}{dt} = \overbrace{\theta \dot{m}_{s,in}}^{Feed} - \overbrace{\gamma \dot{m}_{brine}}^{Brine\ discharge} - n \times \left[A\left(\frac{dq_{ads}}{dt}\right)\right] M_{sg} \tag{4.5}$$

$$M_{s,evap}\frac{dX_{s,evap}}{dt} = \theta X_{s,in}\dot{m}_{s,in} - \gamma X_{s,evap}\dot{m}_{brine} - n \times X_D\left[A\left(\frac{dq_{ads}}{dt}\right)\right] M_{sg} \tag{4.6}$$

where $X_{s,sin}$ and $X_{s,evap}$ are the concentration of the feed and sea water in the evaporator X_D is the concentration of the vapor.

The AD plant comprises of two reactor beds where the adsorbent is packed around the fins and tube of the heat exchanger. Based on the theoretical framework developed, the energy balance of the evaporator in communication with adsorber bed undergoing the adsorption process is written as,

$$\left[M_{s,evap}c_{p,s}\left(T_{evap,}X_{s,evap}\right) + M_{HX,Evap}c_{p,HX}\right]\frac{dT_{evap}}{dt} =$$

$$\theta \times h_f\left(T_{evap}\right)\left[A\left(\frac{dq_{ads}}{dt}\right)\right]M_{sg} +$$

$$\dot{m}_{chilled}c_p\left(T_{evap}\right)\left(T_{chilled,in} - T_{chilled,out}\right) - \gamma \times h_f\left(T_{evap,}X_{s,evap}\right)\dot{m}_{brine} \qquad (4.7)$$

where $M_{HX,Evap}$ is the total mass of the evaporator, M_{sg} is the mass of silica gel, $\dot{m}_{brine}$ is the mass flow rate of brine discharge, q_{ads} denote water vapor uptake by the master adsorption and slave adsorption processes. The first term in the right hand side of Equation 4.7 represents the sensible heat by the supplied feed seawater, the second term stands for the heat removal by the uptake of adsorbent, the third and fourth terms denote the energy supplied by the chilled water and the sensible heat by the brine discharge. The specific heat ($C_{p,s}$) and enthalpy (h_f) of sea water are calculated as functions of temperature and pressure. The vapor pressure depression due to the concentrated salt water is taken into consideration in terms of boiling point elevation (*BPE*). Properties of sea water are given in **Appendix D**. The vapor pressure depression affects the uptake of water vapor by the adsorbent which varies with temperature and the pressure.

The energy balance of the condenser which is in communication with the desorber bed is given by,

$$\left[M_{cond}c_{p,s}(T_{cond}) + M_{HX,cond}c_{p,HX}\right]\frac{dT_{cond}}{dt} =$$

$$-h_f(T_{cond})\frac{dM_d}{dt} + n \times h_{fg}(T_{cond})\left[A\left(\frac{dq_{des}}{dt}\right)\right]M_{sg} +$$

$$\dot{m}_{cond}c_p(T_{cond})\left(T_{cond,in} - T_{cond,out}\right) \qquad (4.8)$$

where $M_{HX,\ cond}$ is the total mass of the condenser and M_d is the mass of distillate extracted from the condenser.

The energy balance Equation of the adsorber bed connected with the evaporator is

$$\left[M_{sg}c_{p,sg} + M_{HX}c_{p,HX} + M_{abe}c_{p,a}(T,P)\right]\frac{dT_{ads}}{dt} =$$

$$\pm n \times \Delta H_{st}(T_{ads}, P_{evap})M_{sg}\frac{dq_{ads}}{dt} \pm$$

$$\dot{m}_{cw/hw}c_p(T_{ads})\left(T_{cw/hw,in} - T_{cw/hw,out}\right) \quad (4.9)$$

The energy balance for the desorber bed is written as,

$$\left[M_{sg}c_{p,sg} + M_{HX}c_{p,HX} + M_{abe}c_{p,a}(T,P)\right]\frac{dT_{des}}{dt}$$

$$= \pm n \times \Delta H_{st}(T_{des}, P_{cond})\frac{dq_{des}}{dt}M_{sg}$$

$$\pm\dot{m}_{cw/hw}c_p(T_{des})\left(T_{cw/hw,out} - T_{cw/hw,out}\right) \quad (4.10)$$

where $T_{cw/hw,out}$ is the outlet water temperature of the master adsorber/desorber bed, ΔH_{st} and $C_{p,a}$ are the isosteric heat of adsorption and the specific heat of the adsorbed phase are is calculated using the expression derived in thermodynamic framework.

Using the heat transfer Equation, the outlet temperature of the water from each heat exchanger is estimated using log mean temperature difference method (LMTD) and it is given by,

$$T_{out} = T_0 + (T_{in} - T_0)\exp\left(\frac{-UA}{\dot{m}c_p(T_0)}\right) \quad (4.11)$$

Where T_o is the temperature of the heat exchanger. The energy required to remove water vapors from the silica gels, here desorption Q_{des} can be calculated using the inlet and outlet temperatures supplied to the reactors, and this is given by,

$$Q_{des} = \dot{m}_{hw} c_p(T_{des})\left(T_{hw,in} - T_{hw,out}\right) \quad (4.12)$$

The energy rejected in an AD cycle to the cooling water by the adsorption process is estimated to be

$$Q_{ads} = \dot{m}_{cw} c_p(T_{ads})\left(T_{cw,in} - T_{cw,out}\right) \quad (4.13)$$

The heat of evaporation Q_{evap} and the condensation energy Q_{cond} rejected at the condenser are given by

$$Q_{evap} = \dot{m}_{chilled} c_p(T_{chilled})\left(T_{chilled,in} - T_{chilled\,,out}\right) \quad (4.14)$$

$$Q_{cond} = \dot{m}_{cond} c_p(T_{cond})\left(T_{cond,out} - T_{cond,in}\right) \quad (4.15)$$

Finally, the performance of the AD cycle is assessed in terms of specific daily water production (SDWP), and the performance ratio (PR) which can be calculated as,

$$SDWP = N \times \int_0^{t_{cycle}} \frac{Q_{cond}}{h_{fg}(T_{cond}) M_{sg}} dt \quad (4.16)$$

$$PR = \int_0^{t_{cycle}} \frac{\dot{m}_d h_{fg}(T_{cond})}{Q_{des}} dt \quad (4.17)$$

where $\dot{m}_d$ is the fresh water production rate in kg/s and N is the number of cycles per day. The SDWP can be expressed as kg of potable water produced per kg of silica gel per day or can also be presented using equivalent expression of m^3 of potable water per tonne of silica gel per day. The performance ratio of the AD cycle is the ratio of the condensation heat to the heat input for desorption.

The above model predicts the performance of different operation modes of the AD cycle of the 2-bed by using the coefficients *A, γ, ε, and θ* of which values are given in **Table B.1 in the Appendix B**. The mathematical modeling equations of the AD cycle will solve using simulation code written in MATLAB, using the input parameters summarized in **Table B.2 in the Appendix B.**

4.2 Simulation Result

For simulation result, the predicted performance of the AD cycle for 2-bed operation mode is calculated from the solution of mathematical modeling. The transient temperature profiles of the major components such as adsorber, desorber, evaporator and condenser of the AD cycle operating as a 2-bed mode are given in Figure 4.1. In the two-reactor mode, one of the beds served as adsorber and the other one as desorber. The predictions show that cyclic steady state is achieved after two half-cycles. The equivalent specific daily water production (SDWP) is estimated to be about 10 m^3/tonne of silica gel per day whilst the production ratio, defined here as the ratio of the latent energy of condensate to the heat input to produce the condensate or PR is about 0.80.

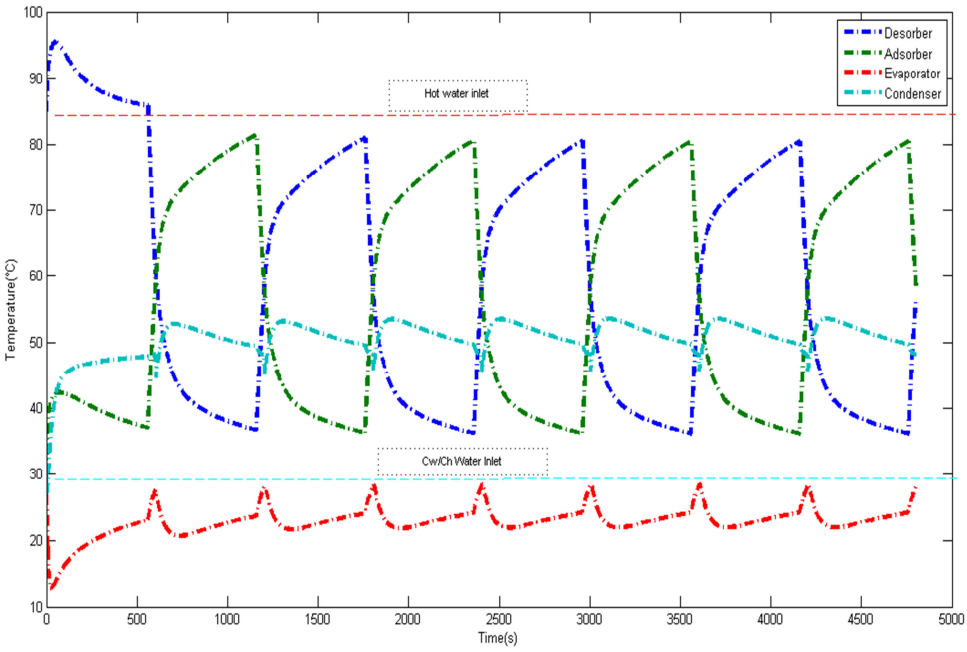


Figure 4.1: The temperature profiles of the major component of the AD cycle operating in 2-bed mode: T_{hw}=85℃, T_{cw}=30℃, T_{ch}=30℃, $F_{hw/cw}$=0.8 kg/s, $F_{chilled}$=0.8 kg/s, $t_{half\text{-}cycle}$=600s, $t_{switching}$=40s

The investigations performances of the AD cycle on the operation cycle time of 2-bed are discussed. In practice, it is obvious that the temperature of the available hot water to operate the AD cycle might not be constant, but it will fluctuate depending on the process from which the waste heat is extracted. On the other hand, desorption

rate is faster for higher temperatures and thus a shorter cycle time may be required to regenerate the water vapor.

Table C.1 in the Appendix C shows the correspondent SDWP and PR with respect to the cycle times and the hot water inlet temperature of adsorption desalination cycle of 2-beds operation modes.

On the basis of optimal conditions (the hot water temperature of 85ºC, operating cycle time 4800s, and the cooling water temperature of 30ºC), the maximum SDWP and PR are obtained as $10m^3$ per tonne of silica gel and 0.80, respectively.

The AD cycle was investigated using different hot water temperatures ranging from 65 ^{o}C to 85^{o}C to evaluate the optimal cycle time at which the cycle gives the highest water production rate. Figure 4.2 shows the SDWP against cycle times for two-bed at different hot water inlet temperatures.

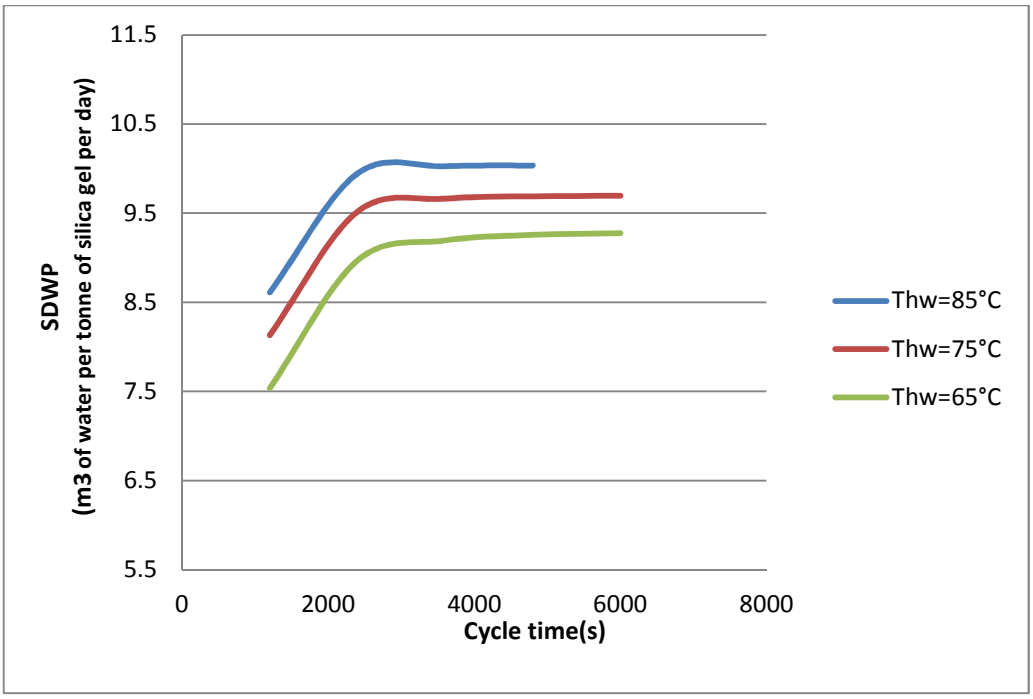


Figure 4.2: SDWP at different cycle times at $T_{hw=}$ 85^{o}C, 75^{o}C, 65^{o}C

These results denote the existence of optimal cycle times at the specific hot water inlet temperature as the SDWP varies with cycle time. Lower SDWP is obtained at relatively shorter cycle times, and this is due to the fact that the regeneration process

during desorption is not completed and the water vapors from silica gels are not fully emitted for condensation and producing water in the condenser. This means that the affinity of the adsorbent (silica gel) for the uptake of water vapor in the next cycle will be damped due to the incomplete regeneration. On the other hand, the lower SDWP at longer cycle time is due to the waste of thermal energy resulting from the excessively longer supply of the hot water to the sorption elements during desorption process. As a result, the additional energy supplied by the hot water has no effect for desorption but just heating the adsorbents and the heat exchanging components. In addition, the total numbers of operation cycles per day is also significantly reduced. The evaluation of the cycle time for different hot water inlet temperatures showed that the longer cycle time is required for lower hot water temperatures.

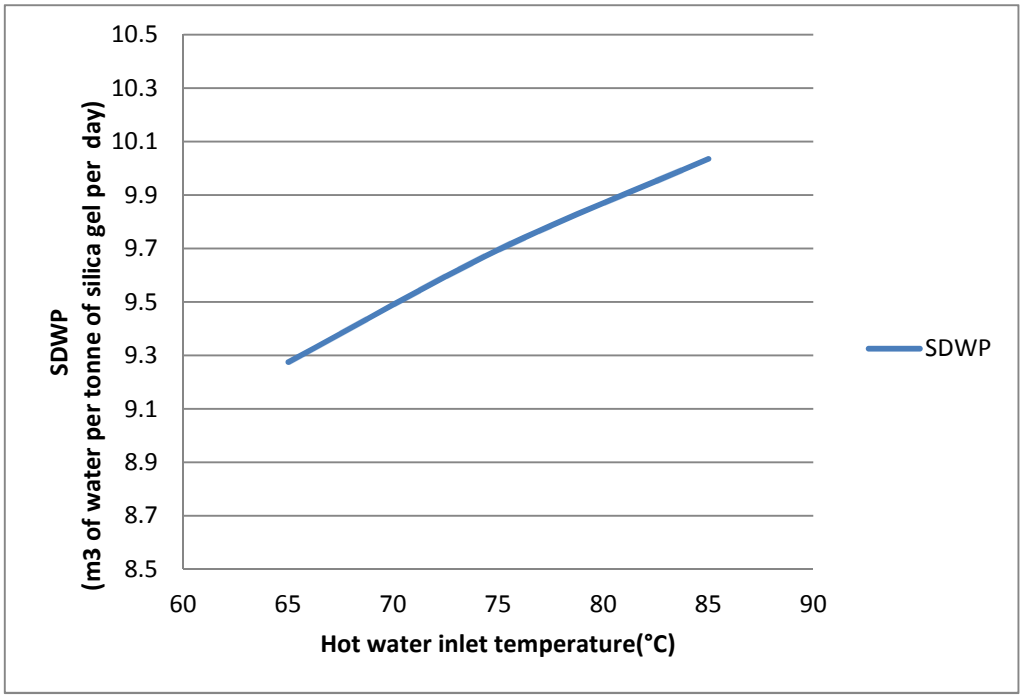


Figure 4.3: SDWP at different hot water inlet temperature range from 65 ^{o}C to 85^{o}C

Figure 4.3 shows the comparison of the specific daily water production of AD cycles operating at two-bed operation modes at respective hot water inlet temperatures. It is noticed that the AD cycle in higher hot water inlet temperatures produces higher SDWP compared with lower hot water inlet temperatures. This is because of fastest regeneration process in the desorption bed at higher inlet temperature.

Meanwhile, the performance of adsorption desalination in terms of performance ratio is investigated based on hot inlet water temperature. Figure 4.4 shows the performance ratio of adsorption desalination cycle in 2 bed operation mode. It is observed that the PR is increased with the increase of hot water inlet temperature. The PR signifies the ratio of the condensation heat to the heat input for desorption. In this 2-bed operation mode, it shows that the condensation heat is higher if the heat input is higher.

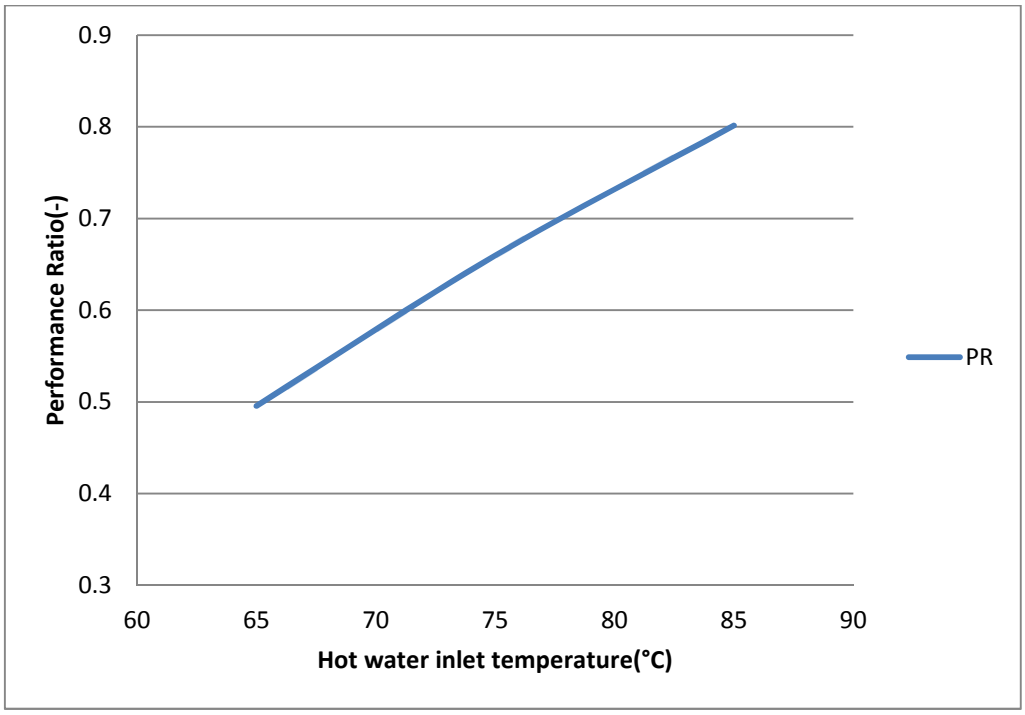


Figure 4.4: Performance Ratio of 2-bed Adsorption Desalination at different hot water inlet temperatures.

CONCLUSION

As a conclusion, this numerical investigation evaluated the performance of adsorption desalination cycle driven by waste heat from industry. The results showed that two-bed mode AD process was capable of producing specific daily water production (SDWP) of 10 m^3 of potable water per tonne of silica gel per day. The optimal cycle time for a specific hot water inlet temperature ranging from 65^{o}C to 85^{o}C for two-bed operation modes was numerically evaluated. The numerical results showed that the operation cycle time for the optimal performance of the AD plant varies with the regeneration temperature of the plant. A longer cycle time is required for lower heat source temperatures in order to completely regenerate subsequently giving the higher water production rate. This work may be applied as a general operation guideline in the adsorption desalination industry where the available heat source temperature may not be at a constant temperature. It will give a large benefit to the world population in producing potable and safe water for daily use. Furthermore, by using this method to produce potable water, it can reduce thermal and electrical energy consumption respectively, and also avoid global warming by using waste heat from the industry.

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APPENDICES

Appendix A: Tools

For numerical investigation on the Adsorption Desalination Cycle, MATLAB and Microsoft Excel will be use to perform all the calculation needed and also producing a graph for graphical representation of data.

A.1) MATLAB

MATLAB is a programming environment for algorithm development, data analysis, visualization, and numerical computation. Using MATLAB, it can solve technical computing problems faster than with traditional programming languages, such as C, C++, and Fortran.

A.2) Microsoft Excel

Microsoft Excel is a commercial spreadsheet application written and distributed by Microsoft for Microsoft Windows and Mac OS X. It features calculation, graphing tools, pivot tables, and a macro programming language called Visual Basic for Applications.

Appendix B: Mathematical Modeling Parameters

Table B.1: Values of the indicators for changing the operation mode of the AD cycle [25]

Mode	Parameter	2-bed mode
Operation	n	2
	θ	1 (charging sea water)
	A	1
	γ	1 (brine discharge)
Switching	n	2
	θ	1 (charging sea water)
	A	0
	γ	1 (brine discharge)

Table B.2: Parameters use in the simulation [25]

Parameters or material properties	Values	Unit	Reference
Sorption thermodynamic properties			
Kinetic constant	2.54×10^4	m^2/s	28
Activation Energy	4.2×10^4	J/mole	28
Average radius of silica gel particle	1.7×10^4	m	Manufacturer
Specific heat of silica gel	921	J/kgK	28

Adsorber bed			
Mass of silica gel per bed	36	kg	Experimental Data
Adsorber/desorber bed heat transfer area (*Abed*)	41.7	m^2	
Tube length	0.576	m	
Number of tubes/cake	15	-	
Number of pass/distribution	30	-	
Thermal mass of adsorber bed including fins and support	284.6	kJ/K	
Overall heat transfer coefficient of adsorber	250	W/m^2 K	
Overall heat transfer coefficient of desorber	180-330	W/m^2 K	
Condenser			
Condenser heat transfer area (A_{cond})	5.08	m^2	
Thermal mass of condenser including fins and support	18.61	kJ/K	
Condenser heat transfer coefficient	2657.5	W/m^2 K	
Mass of condensate in the condenser	10	kg	

Evaporator			Experimental Data
Evaporator heat transfer area (A_{evap})	3.5	m^2	
Evaporator heat transfer coefficient	1715.2	W/m^2 K	
Thermal mass of evaporator including fins and support	25.44	kJ/K	
Mass of refrigerant in the evaporator	250	kg	
Concentration of the feed	35,000	ppm	
Concentration limit to discharge brine	110,000	ppm	

B.3: Numerical Values

$A(T_s) = A0 + A1.T_s + A2.T_s^2 + A3.T_s^3$

$A0$ = -6.5314
A1 = 0.72452E-01
A 2 = -0.23951E-03
A 3 = 0.25493E-06

$B(T_s) = B0 + B1.T_s + B2.T_s^2 + B3.T_s^3$

B 0 = -15.587
B 1 = 0.15915
B 2 = -0.50612E-03
B 3 = 0.53290E-06.

ΔH_{st} = 2.8E+6 J/kg

Appendix C: Simulation Result

Table C.1: Specific daily water production and optimal cycle times at different regeneration temperatures

	SDWP					PR	Max SDWP
Temp/Time	1200s	2400s	3600s	4800s	6000s		
85℃	8.61	9.94	10.02	10.03	-	0.80	10.03
75℃	8.13	9.51	9.66	9.68	9.69	0.65	9.69
65℃	7.53	8.96	9.19	9.25	9.27	0.49	9.27

Appendix D: Properties of Sea Water

1) Vapor pressure of sea water

$$P_{sea} = P_{sat}(T) \times (1 - 5.37 \times 10^{-4} \times S)$$

where *Psea* is the vapour pressure of sea water, *Psat* is the saturation pressure of pure water and *S* is the salinity in ppm.

$$\text{P}sat = 133.32 \times \exp(18.3 - \frac{3820}{T-46.1})$$

2) Boling point elevation

$$BPE = (A + B \times S) \times S$$
$$A = (6.71 + 6.43 \times 10^{-2} \times \text{T} + 9.74 \times 10^{-5} \times \text{T}^2) \times 10^{-3}$$
$$B = (2.38 + 9.59 \times 10^{-3} \times \text{T} + 9.42 \times 10^{-5} \times \text{T}^2) \times 10^{-5}$$

where BPE is the boiling point elevation which is a function of sea water temperature and salinity.

3) Specific heat capacity

$$c_{p,sea} = 2.38846 \times 10^{-4} \times (\text{A1} + \text{A2} \times \text{T} + \text{A3} \times \text{T}^2 + \text{A4} \times \text{T}^3)$$
$$A1 = 4.2068 \times 10^3 - 6.6197 \times \text{S} + 1.2288 \times 10^{-2} \times \text{S}^2$$
$$A2 = -1.1262 + 5.4718 \times 10^{-2} \times \text{S} - 2.2719 \times 10^{-4} \times \text{S}^2$$
$$A3 = 1.2026 \times 10^{-2} - 5.3566 \times 10^{-4} \times \text{S} + 1.8906 \times 10^{-6} \times \text{S}^2$$
$$A4 = 6.8774 \times 10^{-7} + 1.5170 \times 10^{-6} \times \text{S} - 4.4268 \times 10^{-9} \times \text{S}^2$$

4) Specific enthalpy of sea water

$$\text{h}_{sea} = (\text{H}_0 + \text{CPS} \times \text{T}) \times 4186.8$$
$$\text{H}_0 = 2.3\text{D} - 3 \times \text{S} - 1.03 \times 10^{-4} \times \text{S}^2$$
$$\text{CPS} = 2.38846 \times 10^{-4} \times (\text{A1} + \text{A2} \times \text{T} + \text{A3} \times \text{T}^2 + \text{A4} \times \text{T}^3)$$
$$A1 = 4.2068 \times 10^3 - 6.6197 \times \text{S} + 1.2288 \times 10^{-2} \times \text{S}^2$$
$$A2 = -1.1262 + 5.4718 \times 10^{-2} \times \text{S} - 2.2719 \times 10^{-4} \times \text{S}^2$$
$$A3 = 1.2026 \times 10^{-2} - 5.3566 \times 10^{-4} \times \text{S} + 1.8906 \times 10^{-6} \times \text{S}^2$$
$$A4 = 6.8774 \times 10^{-7} + 1.5170 \times 10^{-6} \times \text{S} - 4.4268 \times 10^{-9} \times \text{S}^2$$